

# On the Statistical Significance of Conductance Quantization

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## Abstract

Recent experiments on atomic-scale metallic contacts have shown that the quantization of the conductance appears clearly only after the average of the experimental results. Motivated by these results we have analyzed a simplified model system in which a narrow neck is randomly coupled to wide ideal leads, both in absence and presence of time reversal invariance. Based on Random Matrix Theory we study analytically the probability distribution for the conductance of such system. As the width of the leads increases the distribution becomes sharply peaked close to an integer multiple of the quantum of conductance. Our results suggest a possible statistical origin of conductance quantization in atomic-scale metallic contacts.

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The study of electronic transport through mesoscopic structures has long been a topic of interest. In the last decade much attention has been focused on this subject in connection with the discovery of interesting quantum effects that are directly observable in resistance and conductance experiments. Different phenomena like weak localization [1] and universal conductance fluctuations [2–4] appear as a consequence of electron multiple scattering in the diffusive transport regime. In this regime, the size of the system is larger than the elastic mean free path  $\ell$  but smaller than the phase-coherence length  $L_\phi$ . When the size of the system is reduced further, and becomes less than  $\ell$ , transport is said to be ballistic. The simplest ballistic system is a short, narrow channel connecting two two-dimensional electron gases (2DEG). The conductance of these contacts was shown [5] to be quantized in integer multiples of  $2e^2/h$ , even though the ballistic region is strongly coupled to diffusive structures. This remarkable fact was explained theoretically by Maslov, Barnes and Kirczenov [6] and Beenakker and Melsen [7]. The ballistic constriction between two disordered diffusive leads works as a filter: it suppresses fluctuations and recovers conductance quantization (CQ).

The development of different experimental techniques [8–15] has made it possible to analyze CQ effects in atomic-scale metallic contacts. As the size of the contact is of the order of the electron wave length and much smaller than the elastic mean free path, they provide a natural system to study mesoscopic transport in three dimensional structures. In general, the conductance of these contacts shows complicated plateau-like structures that are not multiples of  $2e^2/h$ . The quantization of the conductance manifests itself only after statistical averaging of different experimental realizations. CQ has been observed as clear peaks at integer multiples of  $2e^2/h$  in the conductance distribution of different metallic contacts. [8–15] The situation could suggest some kind of filtering effect similar to that discussed for a 2DEG ballistic constriction between two diffusive reservoirs.

Motivated by these results we have analyzed a simplified model system in which a narrow neck is randomly coupled to wide ideal leads containing a large number of channels  $N$ . Based on Random Matrix Theory (RMT) [3,16–20] we will show that conductance quantization is an statistical property of the system in the large  $N$  limit. We will study analytically

the probability distribution for the conductance of such system and we will show that it is sharply peaked near the quantum of conductance. We stress that our goal here is to discuss some general statistical properties of the conductance for a model system rather than to fit the experimental results in real atomic-scale contacts.

Our model system is sketched in Fig. 1. The transport properties are characterized by its scattering matrix  $S$  which is usually written in the form

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix},$$

where  $t$  and  $t'$  are the matrices of the transmission amplitudes for the waves incident from the left and from the right respectively. The corresponding matrices of the reflection coefficients are  $r$  and  $r'$ . Flux conservation implies  $S$  unitary while, in the absence of a magnetic field, time reversal invariance requires  $S$  to be symmetric. The conductance of the system, (in units of  $2e^2/h$ ) is given by the two terminal Landauer-Büttiker formula

$$g = Tr(tt^\dagger) = \sum_i T_i, \quad (1)$$

where  $T_i$  are the eigenvalues of  $tt^\dagger$ .

In our model, we assume a random coupling between the channels in the narrow constriction and the wide leads (which are assumed to be perfectly clean). This is in contrast with the usual approach in the 2DEG context, where a ballistic constriction is connected to quasi 1D disordered ohmic wires. As the treatment in terms of RMT makes no reference to dimensionality, the treatment presented in ref. [6,7], based on a Transfer matrix approach, would apply equally well to 3D constrictions connected to ohmic leads. However, the analysis of CQ in metallic contacts presents significant differences.

In atomic-scale metallic contacts the randomness could be associated mainly to the rough walls of the connecting neck between wide and narrow leads [21]. It is worth noticing that for metals there is strong scattering with the constriction walls since the atomic-scale surface roughness is of the order of the electron wavelength. The real situation is even more complicated because of the interplay between mechanical and electrical properties.

[9,24,22,23] The experimental peaks in the histograms are usually obtained after averaging the conductance of the contact under repeated plastic deformation cycles (in which the wide leads remain unchanged). Similar peaks in the conductance histograms have been obtained in numerical simulations of ballistic atomic-scale constrictions [24] connecting two perfectly clean sem infinite leads. In this case the only source of elastic scattering came from the walls of the neck connecting the perfect leads with the narrowest section of the contact. As in the real experiments, the signature of CQ appears only after averaging over different neck geometries. [24]

Based on these physical considerations, we will consider perfect (non ohmic) wide leads randomly connected to a narrow constriction. Since we are interested in a statistical approach, given our limited knowledge of the microscopic coupling between channels, the natural choice of the statistical ensemble is that which maximizes the information entropy subject to the known constraints. In the RMT context, this leads to the circular orthogonal ensemble (COE,  $\beta = 1$ ) in the presence of time-reversal invariance, and to the circular unitary ensemble (CUE,  $\beta = 2$ ) in its absence (for instance, with an applied magnetic field). [16]

We will first analyze the simplest case in which a narrow lead with a few number of conducting channels  $n$  is coupled to a wide one with  $N$  propagating channels (WN geometry) [25]. Following references [17,18], the average ( $\langle g \rangle$ ) and variance ( $var(g) = \langle g^2 \rangle - \langle g \rangle^2$ ) of the conductance can be obtained by averaging on the unitary group,

$$\langle g \rangle = \frac{Nn}{N + n + \delta_{1\beta}} \quad (2)$$

$$var(g) = \frac{\langle g \rangle^2 (1 + \delta_{1\beta})(n + \delta_{1\beta})(N + \delta_{1\beta})}{(Nn)(N + n + 2\delta_{1\beta} + 1)(N + n + \delta_{1\beta} - 1)} \quad (3)$$

From the last expressions it is obvious that conductance quantization is recovered in the case that  $N \gg n$ .

A deeper insight on the statistical properties of  $g$  can be obtained from the complete distribution of the conductance values  $P(g)$ . To compute  $P(g)$  we start from the expression deduced by Brouwer [26] for the distribution of the transmission eigenvalues

$$P(\{T_p\}) \propto \prod_{p < m} |T_p - T_m|^\beta \prod_k T_k^\alpha, \quad (4)$$

with  $\alpha = \frac{1}{2}\beta(|N - n| + 1 - 2/\beta)$ . The probability distribution of the conductance can then be obtained from

$$P(g) = \int \prod_i dT_i \left\{ P(\{T_i\}) \delta(g - \sum_i T_i) \right\}. \quad (5)$$

Although closed expressions for  $P(g)$  can be obtained for small values of  $N$  and  $n$  [18], it is extremely difficult to work it out for larger values. However, a simple analytical expression, for arbitrary  $n$ , can be obtained in the large  $N$  limit.

Let us write the transmission eigenvalues as  $T_k = 1 - \epsilon_k$  ( $\epsilon_k \leq 1$ ). The conductance can then be written as  $g = n - \epsilon$  with  $\epsilon = \sum_k \epsilon_k$ . In the limit  $N \gg n$  (i.e.  $\alpha \gg 1$ ) we have

$$\prod_{k=1}^n T_k^\alpha \sim e^{-\alpha\epsilon}. \quad (6)$$

In terms of  $\epsilon$  the probability distribution is now given by

$$P(n - \epsilon) = e^{-\alpha\epsilon} I(\epsilon) \\ I(\epsilon) = \int \prod_k d\epsilon_k \prod_{i < j} |\epsilon_i - \epsilon_j|^\beta \delta(\epsilon - \sum_m \epsilon_m). \quad (7)$$

If  $\epsilon < 1$  the integration limits of each variable can be extended from zero to infinity showing that  $I(\epsilon)$  is an homogeneous function of degree  $n - 1 + \beta n(n - 1)/2$ . Therefore

$$P(g) \propto e^{-\alpha(n-g)} (n - g)^{n-1+\beta n(n-1)/2}. \quad (8)$$

This distribution is the exact large- $N$  limit in the sense that it reproduces all moments of  $(n - g)$  to the lowest power of  $(1/N)$ .

In Fig. 2 we have plotted  $P(g)$  for different values of  $n$ . The probability is peaked at  $g^*$  close to integer values but slightly shifted downwards,

$$g^* \sim n - (n - 1) \frac{n\beta/2 + 1}{N\beta/2}. \quad (9)$$

As expected, the absence of time reversal invariance (applied magnetic field) ( $\beta = 2$ ) suppresses enhanced coherent backscattering effects, leading to narrower peaks as well as smaller

shifts in the peak positions. Notice also that the quantization “ quality ” of  $P(g)$  is more prominent for larger ratios of  $N/n$  ( this is qualitatively similar to the result obtained within the Transfer Matrix approach [7]).

Let us now consider the wide-narrow-wide (WNW) case in which a narrow neck is randomly coupled to two leads with, in general, different numbers of propagating channels  $N_1$  and  $N_2$  (see Fig. 1). The conductance of the system is now given by

$$g = \text{Tr}[t_1 t_1^\dagger (1 - r_2^\dagger r_1'^\dagger)^{-1} t_2^\dagger t_2 (1 - r_1' r_2)^{-1}], \quad (10)$$

where the 1, 2 index are associated to the coupling with the left and right lead, respectively. The direct averaging of this expression is a formidable task due to the multiple internal reflections. However, in the limit of  $N_{1,2} \gg n$  and to lowest order in  $1/N_{1,2}$  (i.e.  $1/N_1$ ,  $1/N_2$  or  $1/\sqrt{N_1 N_2}$ ), the expression above can be simplified to

$$g = \text{Tr}[t_1 t_1^\dagger + t_2^\dagger t_2 - \mathbf{1} + (r_2^\dagger r_1'^\dagger + r_1' r_2)], \quad (11)$$

where  $\mathbf{1}$  is the  $(n \times n)$  identity matrix. Assuming statistical independence between left and right leads, it can be shown [27] that to leading order, the average and variance of  $g$  are given by

$$\langle g \rangle = n - n(n + \delta_{1\beta}) \left( \frac{1}{N_1} + \frac{1}{N_2} \right) \quad (12)$$

$$\text{var}(g) = (1 + \delta_{1\beta}) n(n + \delta_{1\beta}) \left( \frac{1}{N_1} + \frac{1}{N_2} \right)^2. \quad (13)$$

As in the WN case, the previous expressions guarantee that “ quantization ” is recovered in the large  $N_{1,2}$  limit. This means that the “ filtering ” property of a each WN geometry junction is not degraded by multiple scattering between the wide leads. This intuitively obvious result in the large  $N_{1,2}$  limit can be made rigorous by noticing that the average conductance of the WNW problem is always greater than  $\langle g_1 \rangle + \langle g_2 \rangle - n$ , where  $g_{1,2}$  are the conductances of the left and right WN junctions. [27]

Now we obtain an approximate probability distribution for the complete WNW problem, and show it to be equivalent to classically summing series resistances. Formally, the approximation consist of ignoring the last term in the leading order expression for  $g$  (Eq. 11) ,

whose average (under the assumption of statistical independence) is exactly zero. Therefore we take  $g = g_1 + g_2 - n$ , and the probability distribution follows trivially as the convolution:

$$P(g) = \int dg_1 P_1(g_1) P_2(g - (g_1 - n)), \quad (14)$$

where  $P_{1,2}(g)$  are the probability distributions (eq. 8) for each WN contact. The previous approach admits a simple physical interpretation. First, notice that each isolated WN junction has a conductance  $g_{1,2} = n - \epsilon_{1,2}$ , which translates into the following resistance  $R_{1,2} = n^{-1} + \delta R_{1,2}$  with  $\delta R_{1,2} = \epsilon_{1,2}/n$  (remember  $\epsilon_{1,2} = O(1/N_{1,2})$ ). We can say that  $R_{1,2}$  is the sum of the perfect neck resistance ( $n^{-1}$ ) plus an excess *contact* resistance ( $\delta R_{1,2}$ ) which we can associate with the matching between wide and narrow regions. From a classical point of view, the complete WNW problem can be seen as the series sum of three resistances: the perfect neck resistance plus the two contact resistances:  $R_{series} = n^{-1} + \delta R_1 + \delta R_2$ , with corresponding conductance given by  $g_{series} = n - \epsilon_1 - \epsilon_2 = g_1 + g_2 - n$  (again in the large  $N_{1,2}$  limit). But  $g_{series}$  is precisely the approximate conductance obtained ignoring the last term of Eq. 11, leading directly to the distribution of Eq. 14. This justifies our approximation as corresponding to the classical sum of series resistances. Notice that, unlike the WN case, the previous approach does not reproduce the correct asymptotic large- $N_{1,2}$  distribution. For instance, it gives the correct average (Eq. 12) but underestimates the correct variance (Eq. 13). Nevertheless, we expect it to contain the main qualitative features of the large- $N_{1,2}$  limit. This is seen, for instance, in Fig. 3 where according to (14) the distribution for the WNW case is plotted for different cases. As expected, the trends already present in a single WN contact remain here: decreasing sharpness with increasing  $n/N_{1,2}$ , and different behavior related to the presence or absence of enhanced backscattering ( $\beta = 1, 2$ ).

In conclusion, we have analyzed a simple model system of a quantum point contact within a Random  $S$  Matrix approach, a choice motivated by experimental arguments. Within this model, conductance quantization has an statistical origin. We have studied analytically the probability distribution for the conductance. As a consequence of the random coupling between the narrow and wide leads, we have shown that the conductance distribution presents

peaks at values close to integer multiples of  $2e^2/h$  but slightly shifted to lower values. The conductance peaks become wider (the quantization “quality” degrades) as the number of channels in the contact increases. The absence of time-reversal invariance (produced by appropriate magnetic fields) decreases the deviation from quantized values.

The obtained qualitative behavior (reflected in Figs. 2 and 3) strikingly resembles that observed in actual atomic-scale metallic contacts. The increasing shift and width of the conductance peaks with the number of channels in the contact can be clearly seen in the experimental conductance histograms [8–15]. Our results suggest a possible statistical origin of conductance quantization in atomic-scale metallic contacts.

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## FIGURES

FIG. 1. Sketch of our model system for the wide-narrow-wide (WNW) geometry analyzed in the text.

FIG. 2. Conductance probability distribution  $P(g)$  for a WN geometry for  $N = 50$  and different number of channels in the narrow lead ( $n = 1 - 4$ ). Dashed (solid) line corresponds to  $\beta = 1$  ( $\beta = 2$ ).

FIG. 3. Conductance probability distribution  $P(g)$  for a WNW geometry for  $N_1 = 40$ ,  $N_2 = 60$  and different number of propagating modes in the neck ( $n = 1 - 4$ ). Dashed (solid) line corresponds to  $\beta = 1$  ( $\beta = 2$ ).

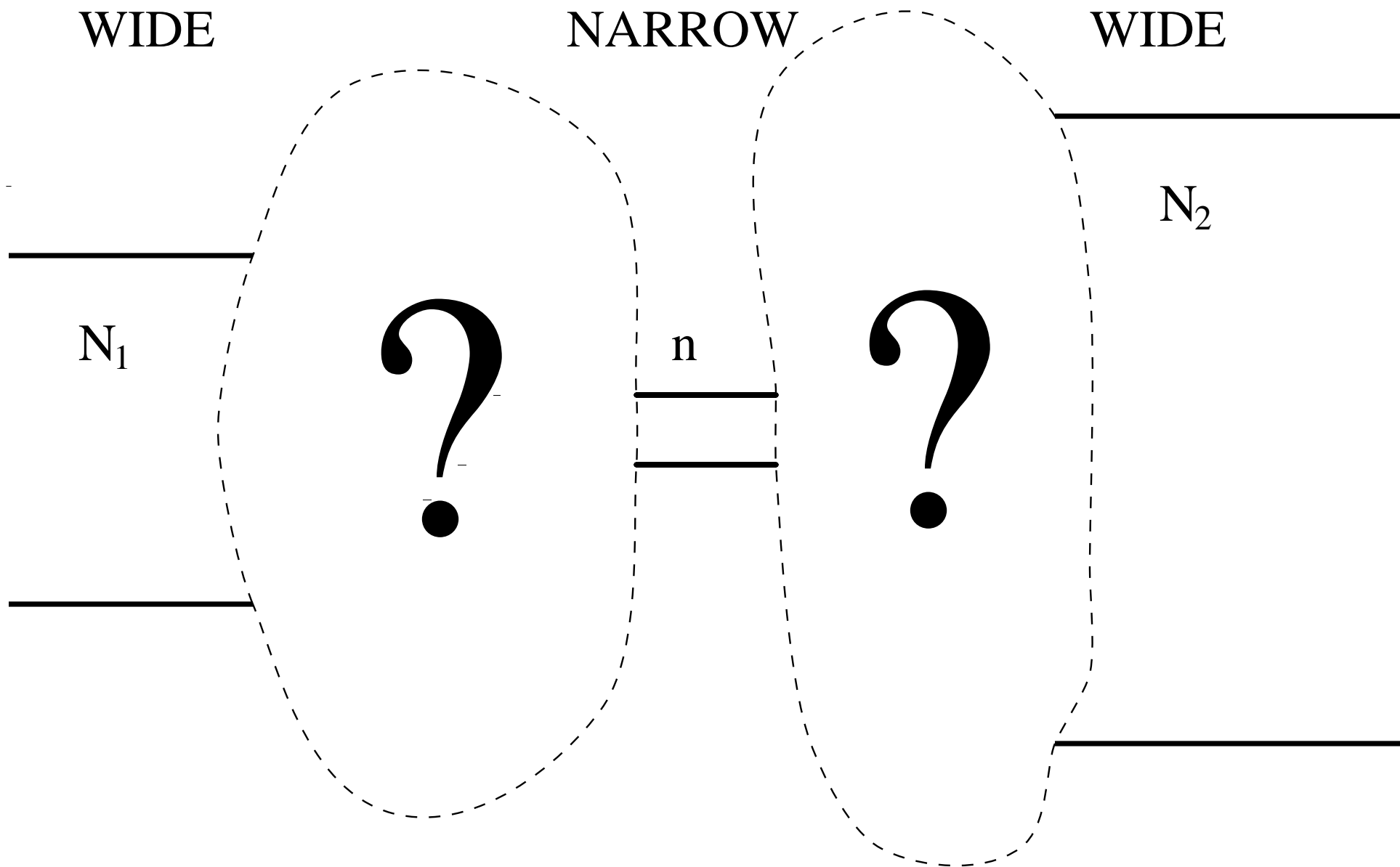


FIGURE 2, BASCONES ET AL, PRB (RC)

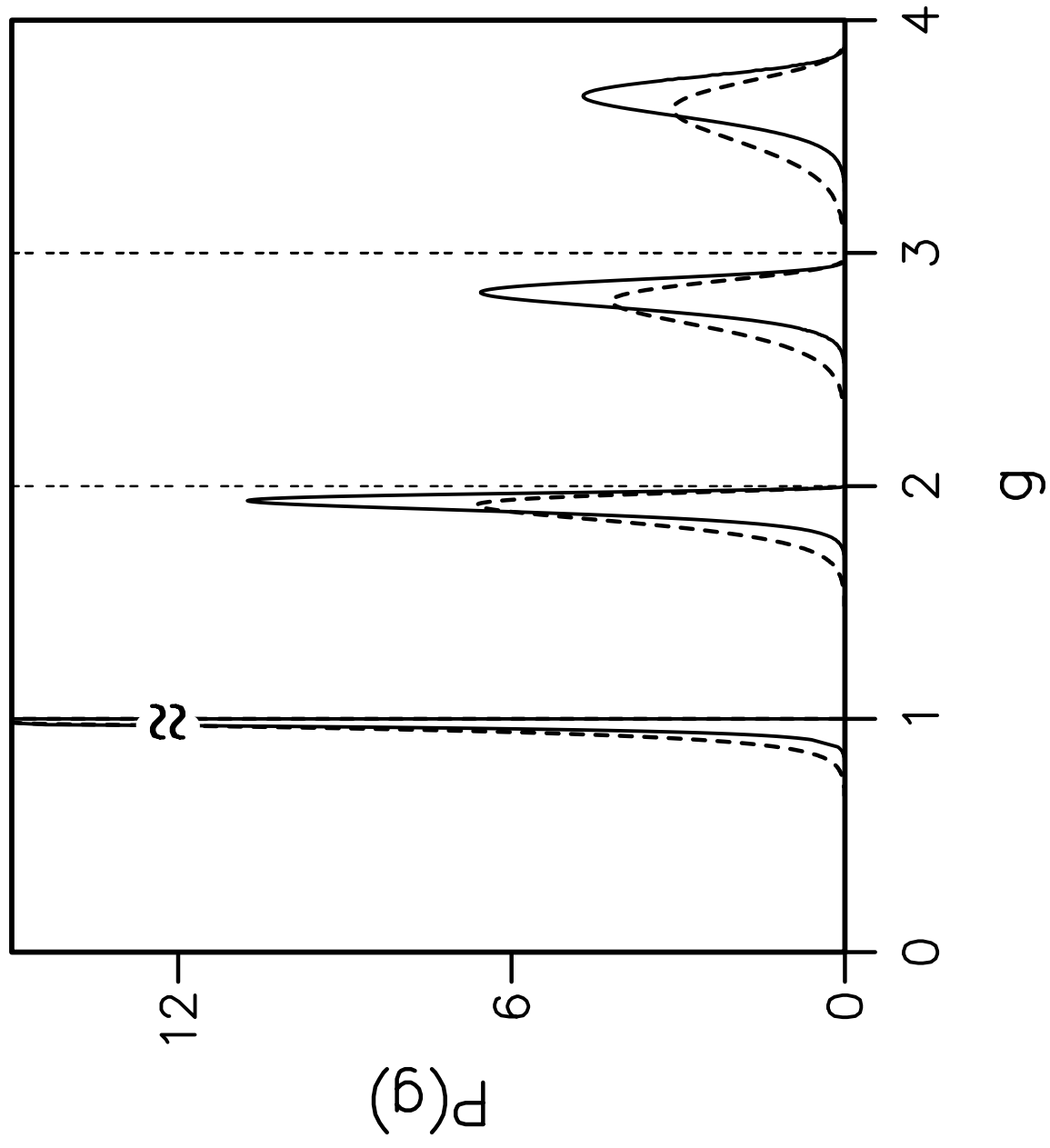


FIGURE 3, BASCONES ET AL, PRB (RC)

